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# Outdoor Chamber Study to Test Multi-Day Effects
# Volume 3. Documentation for Computer-Readable Environmental Chamber Data

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# OUTDOOR CHAMBER STUDY TO TEST MULTI-DAY EFFECTS

## VOLUME III. COMPUTER-READABLE ENVIRONMENTAL CHAMBER DATA

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16. ASSTRACT

The smog chamber facilities of the University of California, Riverside were used to collect experimental data to assess the effects of multi-day irradiations on photochemical oxidant formation. This volume includes documentation on the computer-readable magnetic tape that contains all the data collected in the study. The tape is suitable for use by modelers to develop and test kinetic mechanisms of photochemical smog formation.

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## ABSTRACT

A series of single- and multi-day indoor and outdoor environmental chamber experiments have been carried out at the Statewide Air Pollution Research Center (SAPRC) at the University of California in Riverside to derive data suitable for testing chemical models for multi-day photochemical air pollution episodes. Two environmental chambers were used during this program, a ~6400-ℓ indoor Teflon chamber with blacklight irradiation and a ~50,000-ℓ dual-mode outdoor Teflon chamber which employed natural sunlight as the light source. A total of 32 indoor and 55 outdoor chamber experiments were completed during this program. These chamber experiments consisted primarily of multi-day $NO_x$-air irradiations of an eight-component hydrocarbon surrogate designed to represent emissions of reactive organics into urban atmospheres from all sources, and associated control and characterization runs. Most of the multi-day surrogate-$NO_x$-air experiments in the outdoor chamber were run with the chamber in the dual mode, where each experiment consisted of simultaneous irradiation of two different mixtures under the same temperature and lighting conditions. In addition, an isobutene-$NO_x$-air irradiation was carried out in the indoor chamber to test chemical computer models for the $NO_x$-air reactions of this surrogate component.

Problems with side inequivalency in the dual-mode outdoor chamber experiments were encountered in preliminary experiments carried out in 1982. These were subsequently resolved, and good side-to-side equivalency was obtained in the experiments carried out in 1983. During that time, irradiations of a "standard" surrogate-$NO_x$-air mixture were carried out under a variety of temperature and light intensity conditions, allowing the combined effects of these to be determined. Good reproducibility of experiments carried out under similar weather conditions was observed.

The multi-day surrogate-$NO_x$-air irradiations were carried out in both chambers at a variety of initial hydrocarbon and $NO_x$ concentrations. In general, it was found that runs which were less reactive on the first day with respect to $O_3$ formation tended to be more reactive on subsequent days, and vice-versa. This resulted in the maximum $O_3$ levels in multi-day runs being much less dependent on initial reactant concentrations than expected based on results of single-day irradiations.

The data obtained during this program are presented in three volumes, of which this is Volume III. In Volume I, the experimental facility, methods of procedure, and analytical techniques are described, and the results are summarized and discussed. Volume II contains printouts of the detailed data from these experiments, and this volume contains the data in computer-readable format. These volumes are submitted in fulfillment of Cooperative Agreement No. CR810260-01 for the U. S. Environmental Protection Agency, which covers the period from August 11, 1982 through August 10, 1984.

CONTENTS


| | Page |
|---|---|
| Abstract | iii |
| Tables | vi |
| Acknowledgement | vii |
| I. Introduction | 1 |
| II. Data Tabulations for the Indoor Chamber Experiments | 8 |
| III. Data Tabulations for the Outdoor Chamber Experiments | |

TABLES


| Number | | Page |
|---|---|---|
| 1 | Run Numbers and Run Types for All Indoor Chamber Runs on the Data Tape | 2 |
| 2 | Run Numbers and Run Types for All Outdoor Chamber Runs on the Data Tape | 3 |
| 3 | Organization of Data Files for Chamber Runs | 8 |

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# SECTION I

## INTRODUCTION

In order to obtain an experimental data base required for the development and testing of chemical kinetics mechanisms for multi-day air pollution episodes, the Environmental Sciences Research Laboratory of the U. S. Environmental Protection Agency contracted to the Statewide Air Pollution Research Center of the University of California, Riverside, to carry out a series of indoor and outdoor environmental chamber experiments simulating multi-day conditions using hydrocarbon and $NO_x$ mixtures designed to represent those present in urban airsheds, along with appropriate control and characterization runs. A description of the experimental facility, procedures and analytical techniques, and a summary and discussion of the results obtained are given in Volume I of this three-volume report, and in Volume II, the detailed tabulations of the data are presented. In this volume, the data are given on tape on magnetic tape in computer-readable format.

The computer tape associated with this volume consists of a total of 83 files, each file giving the data from a single experiment. The data density is 1600 BPI, the maximum block size is 8000 bytes, with each block consisting of up to 100 80-byte logical records, and the character format is EBCDIC. Tables 1 and 2 give the tape file number, the indoor or outdoor chamber run number and an indication of the type of run for each run included on the data. Gaps in the sequence of run numbers correspond to runs which are $NO_2$ actinometry experiments (for which tabulations are not given - see Volume I for the results of these experiments), runs for other programs or runs which were aborted. The organization of the individual data sets is described in Section II of this volume.

Table 1. Run Numbers and Run Types for All Indoor Chamber Runs on the Data Tape

| Tape File No. | ITC Run No. | Run Type |
|---|---|---|
| 1 | 621 | $NO_x$-air |
| 2 | 623 | Propene-$NO_x$ |
| 3 | 624 | $O_3$ dark decay |
| 4 | 625 | $NO_x$-air + CO-$NO_x$-air |
| 5 | 626 | 4 ppmC surrogate-0.3 ppm $NO_x$ (2-day) |
| 6 | 627 | Acetaldehyde-air |
| 7 | 628 | $NO_x$-air + CO-$NO_x$-air |
| 8 | 630 | 2 ppmC surrogate-0.3 ppm $NO_x$ (3-day) |
| 9 | 631 | 1 ppmC surrogate-0.3 ppm $NO_x$ (3-day) |
| 10 | 632 | Acetaldehyde-air |
| 11 | 633 | 4 ppmC surrogate-0.6 ppm $NO_x$ (3-day) |
| 12 | 634 | $NO_x$-air + CO-$NO_x$-air |
| 13 | 635 | 4 ppmC surrogate-1.2 ppm $NO_x$ (2-day) |
| 14 | 636 | Acetaldehyde-air |
| 15 | 637 | 4 ppmC surrogate-0.3 ppm $NO_x$ (4-day) |
| 16 | 638 | $NO_x$-air + CO-$NO_x$-air |
| 17 | 639 | Acetaldehyde-air |
| 18 | 640 | $O_3$, $O_3$ + $NO_x$ irradiation |
| 19 | 641 | $O_3$ dark decay |
| 20 | 642 | Pure air irradiation |
| 21 | 643 | Polluted air irradiation |
| 22 | 644 | Polluted air + $NO_x$ irradiation |
| 23 | 690 | Propene-$NO_x$ conditioning |
| 24 | 692 | $NO_x$-air |
| 25 | 693 | Propene-$NO_x$ |
| 26 | 694 | Isobutene-$NO_x$ |
| 27 | 695 | $NO_x$-air |
| 28 | 697 | $O_3$ dark decay |

Table 2. Run Numbers and Run Types for All Outdoor Chamber Runs on the Data Tape

| Tape File No. | OTC Run No. | Run Type |
|---|---|---|
| 1982 Series | | |
| 29 | 146 | Acetaldehyde-air |
| 30 | 147 | $O_3$ dark decay |
| 31 | 148 | Propene-$NO_x$ |
| 32 | 149 | Pure air vs. CO-air |
| 33 | 150 | $NO_x$-air vs. CO-$NO_x$-air |
| 34 | 151 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 35 | 152 | $NO_x$-air (divided chamber) |
| 36 | 153 | Surrogate-$NO_x$ (undivided chamber) |
| 37 | 155 | $NO_x$-air (divided chamber) |
| 38 | 157 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 39 | 158 | $O_3$ dark decay |
| 40 | 159 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test) |
| 41 | 160 | $NO_x$-air (divided chamber) |
| 42 | 161 | Pure air irradiation |
| 43 | 162 | $NO_x$-air in previously irradiated pure air (divided chamber) |
| 44 | 163 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 45 | 165 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test with sides reversed) |
| 46 | 166 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test with modified background) |
| 47 | 167 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test with modified foreground) |
| 48 | 168 | $NO_x$-air (divided chamber) |
| 49 | 169 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test) |

(continued)

Table 2 (continued) - 2

| Tape File No. | OTC Run No. | Run Type |
|---|---|---|
| 50 | 170 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test with rotated frame) |
| 51 | 171 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test with rotated frame and sides reversed) |
| 52 | 172 | Propene-$NO_x$ conditioning |
| 53 | 173 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test) |
| 54 | 174 | Propene-$NO_x$ conditioning |
| 55 | 175 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test in new location) |
| 56 | 176 | Ozone dark decay |
| 57 | 177 | Propene-$NO_x$ conditioning |
| 58 | 178 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test) |
| 59 | 179 | Propene-$NO_x$ vs. propene-$NO_x$ (side equivalency test) |
| 60 | 181 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 61 | 182 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 1983 Series | | |
| 62 | 183 | $O_3$ dark decay |
| 63 | 185 | $NO_x$-air |
| 64 | 186 | Propene-$NO_x$ conditioning |
| 65 | 187 | $NO_x$-air + CO-$NO_x$-air |
| 66 | 188 | $NO_x$-air + CO-$NO_x$-air |
| 67 | 189 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 68 | 190 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test with sides reversed) |

(continued)

Table 2 (continued) - 3

| Tape File No. | OTC Run No. | Run Type |
|---|---|---|
| 69 | 191 | Propene-$NO_x$ conditioning |
| 70 | 192 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 71 | 194 | Surrogate-$NO_x$: variable surrogate |
| 72 | 195 | Surrogate-$NO_x$: variable surrogate |
| 73 | 196 | Surrogate-$NO_x$ (day 1); surrogate-$NO_x$ vs. acetaldehyde-air (day 2) |
| 74 | 197 | Surrogate-$NO_x$: variable $NO_x$ |
| 75 | 198 | Surrogate-$NO_x$: variable surrogate and $NO_x$ |
| 76 | 199 | Surrogate-$NO_x$ vs. surrogate-$NO_x$ (side equivalency test) |
| 77 | 200 | Acetaldehyde-air (divided chamber) |
| 78 | 201 | $NO_x$-air + CO-$NO_x$-air (divided chamber) |
| 79 | 202 | Surrogate-$NO_x$: variable $NO_x$ and surrogate |
| 80 | 203 | Surrogate-$NO_x$: variable $NO_x$ |
| 81 | 204 | Surrogate-$NO_x$: variable $NO_x$ |
| 82 | 205 | Surrogate-$NO_x$: variable $NO_x$ |
| 83 | 206 | Acetaldehyde-air (divided chamber) |

## SECTION II

## ORGANIZATION OF THE DATA SETS

The environmental chamber data are organized into data files, with the results of each indoor or outdoor chamber experiment given in a separate file. The data files consist of records in card image format, which are organized as indicated in Table 3. The following points should be noted regarding these data sets:

- Because this data format is used for a number of different types of experiments at SAPRC, the records contain provisions for data values which are not used in these particular runs. These should be ignored; usually (but not always) they are zero.
- The types of data on the data sets can be categorized by (a) general information data, such as run title, date, number of instruments, comments, chambers, etc., (b) comments, (c) instrument descriptions, (d) channel parameters and (e) channel data. By "channel" we mean the set of experimental measurements which depend on time, such as ozone concentrations, temperature readings, etc.
- Most channels which have data have associated with them a "time set," which is an array of the times at which the measurements for that channel were made. The time sets are stored separately from the channel data because in general more than one channel may have the same time set.
- For outdoor runs 172, 175 and 185-206 (excluding aborted or dark runs), there are two separate channels for the data from the UV radiometer. The channel labeled "UV RAD" consists of the 10-minute averages of the detailed data, while the detailed data, obtained by digitizing the radiometer strip charts using a manual digitizer, are associated with the channel labeled "UV-RAD." The "UV RAD" data are stored in the data sets in the normal manner, but the detailed "UV-RAD" data and their measurement times appear at the end of the data sets, as indicated in Table 3. For the other chamber runs, detailed radiometer data are not available; for most of these runs, the data are available as six-minute averages and are stored on the data sets as a regular channel.

- For outdoor chamber runs, data taken when sampling the air from outside the chamber are always designated as "side 3," even if the chamber was not divided. "Side 1" and "side 2" refer to the chamber side from which the air for sampling was withdrawn, regardless of whether the chamber was divided. If no side number is given for a particular channel, the data applies to both sides (e.g., light intensity data, background measurements, etc.).

- T = 0 refers to the clock time at which the irradiation began; or, for dark runs, the time the first measurement was made.

- In some cases, channels appear on these data sets which do not appear on the printouts in Volume II of this report. These all have "print orders" (PRTORD in group 3 or Table 3) of 8000 or greater. These include the NO and $NO_2$ measurements in the flow tube used to measure the $NO_2$ photolysis rate (the K1 channel), and measurements from instruments whose data was subsequently judged to be unreliable and whose data were rejected (PRTORD $\geq$ 9000).

- Some data points are "flagged" with a non-blank character (as indicated by the values in the "LFLGS" and "FLGS arrays in group 3 of Table 3), which associates it with a comment which has the same character as its associated flag ("FLGCOM" in group 5 of Table 3). These comments indicate problems, etc., with the "flagged" data point, or set of data points starting with the one which is flagged. If a comment has FLGCOM = "N," the comment line is a continuation of the previous flagged comment, and the character "N" does not appear on the printouts in Volume II.

Table 3. Organization of the Data Files for Chamber Runs

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| Group 1. Four Records. General Information | | | | |
| 1 | 1-7 | (1X,I6) | IRUNID | Run number + 1000 x chamber number (chamber numbers: 2 = ITC, 4 = OTC) |
| | 8-13 | (I6) | FORM | File format; always 1. |
| | 14-29 | (A16) | UPDRUN | Date of last update (internal SAPRC use) |
| | 30-69 | (A40) | TITLE | Run title |
| | 70-77 | (A8) | DATE(1) | First half of run date |
| 2 | 1-9 | (1X,A8) | DATE(2) | Second half of run date |
| | 10-25 | (I6) | TZERO | Clock time at T = 0 |
| | 16-21 | (I6) | PSTPDT | 1 for PST, 2 for PDT |
| | 22-39 | (3I6) | - | (Ignore) |
| | 40-45 | (I6) | BAGNO | ITC or OTC reaction bag number |
| | 46-78 | (3G11.4) | - | (Ignore) |
| 3 | 1-57 | (1X,6E11.4) | - | (Ignore) |
| | 50-64 | (I7) | - | (Ignore - should be zero) |
| | 65-70 | (I6) | NSIDES | Number of sides if chamber is divided (Note: "Side 3" always refers to ambient air outside chamber.) |
| 4 | 1-7 | (1X,I6) | NTS | Number of time sets |
| | 8-13 | (I6) | NCHN | Number of channels |
| | 14-19 | (I6) | - | (Ignore - should be zero) |
| | 20-25 | (I6) | NINS | Number or instruments |
| | 26-31 | (I6) | NCOMS | Number of comments |
| | 32-37 | (I6) | - | (Ignore) |
| | 38-48 | (E11.4) | - | (Ignore) |
| | 49-54 | (I6) | - | (Ignore) |
| Group 2. One Set of One or More Records for Each of the NTS Time Sets | | | | |
| 1 | 1-7 | (1X,I6) | NPTS | Number of points in this time set |
| | 8-73 | (11I6) | TIMES | Clock times + 10000 x day number. (Day number: 0 = first day, 1 = second day, etc. E.G., 10930 = 9:30 AM on day 2 of the run.) |

(continued)

Table 3. (continued) - 2

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| 2+ | 1-73 | (1X,12I6) | TIMES | Rest of clock times. (No records of this type if NPTS ≤11.) |
| Group 3. | One Set of Three or More Records for Each of the NCHN Data Channels | | | |
| 1 | 1-7 | (1X,I6) | ID1 | Data type identification number (internal SAPRC use). |
| | 8-13 | (I6) | INST | Instrument number - I.E. record number in group 4 that describes the instrument used for this channel. (0 = instrument undefined) |
| | 14-19 | (I6) | SIDE | Side number (3 = outside). Ignore if NSIDES = 0 or 1. |
| | 20-25 | (I6) | TIMSET | Time set number. (If TIMSET = 0 and PRTORD (see below) = -2, then data for this channel is read in separately as group 5. For these runs, this is the case only for "UV-RAD" channels in the outdoor runs. If TIMSET = 0 and PRTORD ≠ -2, there is no data for this channel.) |
| | 26-31 | (I6) | NP | Number of data points (ignore if TIMSET = 0) |
| | 32-37 | (I6) | NF | Number of flagged data points (Ignore if TIMSET = 0) |
| | 38-67 | (5I6) | - | (Ignore) |
| | 68-73 | (I6) | PRTORD | If >0, determines order channel appears on printouts - lower number printed first. If PRTORD = -2, channel is printed separately at end of printouts, in a format appropriate for channels with an unusually large number of data points. (See also description of TIMSET, above, for further considerations if PRTORD = -2. |
| | 74-79 | (I6) | DIG | (DIG-2) = number of digits to the right of the decimal point that appears on printouts. If DIG = ≥0 or ≤7, data prints out in exponential notation. |

(continued)

Table 3. (continued) - 3

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| 2 | 1-7 | (1X,I6) | UNTS | Code number for units of data: 1 = ppm, 2 or 9 = degree C, 7 = mw-cm$^{-2}$, 10 = degree F, 13 = "raw data," 16 = min$^{-1}$ |
| | 8-19 | (2I6) | - | (Ignore) |
| | 20-41 | (2E11.4) | FAC,ZERO | Factor and zero corrections. Data values = factor x (raw data - zero) (Note however that data values stored on the data sets are already calculated, so these quantities can be ignored.) |
| | 42-52 | (E11.4) | - | (Ignore) |
| | 53-63 | (E11.4) | CONCØ | Initial concentration (if SDEV, below, <0) or average (if SDEV ≥0) to appear at the start of the printouts. If CONCØ = -9.9999E+9, initial concentration or average is not used. If CONCØ = -9.9999E+9, it needs to be calculated from the data. |
| | 64-74 | (E11.4) | SDEV | If SDEV <0, CONCØ is an initial concentration. If SDEV = -1, the initial concentration was assigned; if SDEV = -9.9999E+9, the data value at T = 0 is used as the initial concentration. If SDEV ≥0, CONCØ is the average of the data, and SDEV is the (1σ) standard deviation. If SDEV = 9.999E+9, the standard deviation is unknown. |
| 3 | 1-9 | (1X,A8) | NAME | Channel name |
| 4+ | 1-78 | (1X,7E11.4) | DATA | The data values. As many records as needed for the NP values. A data value of 9.9999E+9 means no data is available for that time point. No records if TIMSET = 0. |

(continued)

Table 3. (continued) - 4

| Record | Column | Format[a] | Name | Description |
|---|---|---|---|---|
| 5+ | 1-73 | (1X,9(I6,A2)) | LFLCS, FLGS | For each of the NF flagged data points, LFLGS is the index number for the point, and the first byte of FLGS is the flag character. As many records as needed for the NF values; no record if NF = 0. |
| Group 4. One Record for Each of the NINS Instruments | | | | |
| 1 | 1-7 | (1X,I6) | INSCOD | Instrument code number |
| | 7-19 | (6A2) | - | (Ignore) |
| | 20-27 | (A8) | INSLBL | Instrument label |
| | 28-67 | (A40) | INSDSC | Instrument description |
| | 68-78 | (E11.4) | - | (Ignore) |
| Group 5. One Record for Each of the NCOMS Comments | | | | |
| 1 | 1-3 | (2X,A1) | FLGCOM | If blank, the comment appears on the first page of the printouts. If not blank, the comment is a footnote which is printed along with the first byte of FLGCOM at the end of the printout. |
| | 4-80 | (A77) | COMENT | The comment line |
| Group 6. Detailed Radiometer Data. These Records Only Appear if One of the Channels (Always "UV-RAD" for These Runs) has PRTORD = -2 and TIMSET = 0. First Record Determines How Many Subsequent Records. | | | | |
| 1 | 1-5 | (I5) | NPTS | Number of data points |
| 2+ | 1-20 | (10X,F10.3) | TIME | Clock time. Data to left of decimal point has same meaning as in the/integer clock time values read in group 2. Data to right of decimal point is fraction of a minute. (E.G., 10930.500 = 30 seconds after 9:30 AM on day 2) |
| | 21-40 | (10X,F10.3) | DATA | Data values. |

[a]FORTRAN format code.

Table 3. Representative Abbreviations Used in the Data Tabulations

| Abbreviation | Meaning |
|---|---|
| $NO_2$-UNC | $NO_2$ readings, uncorrected for interferences by organic nitrates and $HNO_3$ |
| N-C4 | n-Butane |
| I-C4 | Isobutane |
| ISO-C8 | Iso-Octane (2,2,4-trimethylpentane) |
| I-C4= | Isobutene |
| M-XYL | m-Xylene |
| C5-K-3 | 3-Pentanone (diethyl ketone) |
| C5-N-2 | 2-Pentyl nitrate |
| ACETALD | Acetaldehyde[a] |
| MEK | Methyl ethyl ketone[a] |
| PROX | Propene oxide[a] |
| BUTYRAL | Butyraldehyde[a] |
| LN C4/C3= | ln([n-butane]/[propene]), whose rate of change is used to derive OH radical concentrations[b] |
| DEW PT | Dew point (units of degrees C) |
| K1 | $k_1$, the $NO_2$ photolysis rate (units of $min^{-1}$) |
| UV-RAD | UV radiometer readings (units of mW $cm^{-2}$) |

[a]Or some other compound with the same retention time on the gas chromatographic system employed.

[b]Concentration units are arbitrary; only the slope of the log is of interest.